

B25 The Simultaneous Detection of Rodenticides and Drugs Using Thermal Desorption Direct Analysis in Real-Time Mass Spectrometry (TD/DART[®]-MS)

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Learning Overview: After attending this presentation, attendees will better understand Thermal Desorption Direct Analysis in Real-Time Mass Spectrometry (TD-DART[®]-MS) for the analysis of drug evidence suspected of containing superwarfarins, such as rodenticides. Attendees will be presented with instrument optimization parameters, representative spectral analysis and sensitivities, and a discussion of the effect of competitive ionization on the identification of these compounds in complex mixtures and examples of detection of these compounds in street samples.

Impact on the Forensic Science Community: The presentation will impact the forensic science community by providing key information for the use of TD-DART-MS for the analysis and simultaneous detection of rodenticides and drugs, such as cocaine, methamphetamine, heroin, and synthetic cannabinoids.

As drug analysis becomes increasingly complex, due to the onslaught of novel psychoactive substances (NPSs), drug chemists are being tasked to analyze more complex drug mixtures. These analyses are further complicated when additional toxic components are added to street drug samples. One class of compounds that has been reported in the past and is being encountered more frequently is rodenticides, also known as superwarfarins. These compounds, which are the active ingredient(s) in rodent poisoning, cause severe bleeding in drug users which can lead to death. In April 2018, the Centers for Disease Control (CDC) released a warning on synthetic marijuana containing these compounds and others have reported these compounds in cocaine and other drugs. More recently, the FDA also issued a warning about the health hazards of contaminated illegal synthetic cannabinoid products. While these compounds can be detected by techniques such as gas chromatography mass spectrometry (GC/MS), forensic analysts could benefit from a rapid tool to screen drug samples for superwarfarins, both for the purposes of casework and to provide information to trigger a public health response.

Direct analysis in real-time mass spectrometry (DART-MS) is an ambient ionization mass spectrometry technique that has been gaining popularity in forensic analyses due to its ease of use, minimal sample preparation, and rapid (less than 5 seconds) analysis times. DART-MS has also been shown to be able to detect a range of compounds from drugs to explosives to paints and lubricants. However, one of the concerns with traditional DART-MS analysis is the potential exposure to aerosolized sample via inhalation. This work utilizes a variant of DART-MS, thermal desorption direct analysis in real-time mass spectrometry (TD-DART-MS), which minimizes this risk by confining the region of sample introduction and the flow of subsequent aerosolized particles.

This work focused on the use of TD-DART-MS for the detection of rodenticides present in drug mixtures. The study was comprised of method development for these compounds, understanding the mass spectral response and sensitivity and also understanding the competitive ionization effects that can occur when complex mixtures of rodenticides and drugs are analyzed. A total of six rodenticides (bromadiolone, brodifacoum, chloropacinone, difenacoum, diphacinone, and pindone) were investigated. Method development included optimization and understanding the effects of the DART gas (N₂ vs He), the sample desorption temperature, and the Vapur flow rate as well as comparing these settings to those previously established for drug analysis. From the optimized method, representative spectral responses were collected and, as expected, the protonated molecular ion was most often found to be the predominant ion, except for Bromadiolone which had a predominant dehydroxylated molecular ion. Limits of detection were all determined to be less than 100 ng. Competitive ionization studies show minimal effects when the rodenticide is present at greater than 5 % of the mixture. Current work focusses on the ability to screen real case samples for rodenticides, providing forensic practitioners with a rapid method of screening samples that can be done safely and at the low levels required.

Rodenticides, DART[®]-MS, Drug Analysis

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